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Note

On Numerical Differentiation on a Nonuniform Grid

It is well known that if the mth derivative of a function $F(x)$ is approximated with the values of F at k ($>m$) points $x_1, x_2, \ldots, x_k$, the maximum accuracy attainable is in general of order h^{k-m} if h is of the order of the typical distance between pairs of points [1]. For instance, if the first derivative at point x_A, $F'(x_A)$, is estimated in terms of the values of F at x_A, x_B, x_C we have

$$F'(x_A) = \frac{(x_C - x_A)^2[F(x_B) - F(x_A)] - (x_B - x_A)^2[F(x_C) - F(x_A)]}{(x_B - x_A)(x_C - x_A)(x_C - x_B)} + O(h^2). \quad (1)$$

On a nonuniform mesh, formulas such as this one may cause numerical difficulties when two points are so close together that the denominator becomes small. Another difficulty is encountered when one (or more) points move, for instance, against a fixed grid, for in this case the magnitude of the denominator cannot be controlled by a suitable layout of the initial grid spacing. An obvious remedy for such a problem is the prescription that if B, for instance, becomes too close to A, then another point, B', should be used in place of B in this formula. The problem here is more subtle, but may be just as severe since the sudden shift from the triple (A, B, C) to (A, B', C) may introduce inaccuracies and dangerous perturbations in the calculation.

In this note we wish to discuss an alternative procedure which has been found to be very satisfactory. While actual numerical results will be discussed in a forthcoming paper on potential flows with a free surface [2], in view of its general applicability and usefulness, it seemed appropriate to present the basic concept in the present note directed to a wider audience.

Essentially, the idea is to *make use of* $(k+1)$, *rather than* k, *points not to increase the accuracy, but to eliminate the aforementioned problems.* For ease of exposition we shall refer to a particular example with a simple physical content. Extensions and generalizations are immediate.

Consider the problem of a material point in rectilinear motion under the action of a conservative force described by the potential $F(x)$. Suppose that the potential is known on a grid of points of uniform spacing h, and at the position occupied by the material point itself. The problem is to evaluate the force $F'(x)$ at the position x_P occupied by the material point using the values of F ar $x_P, x_B, x_C, \ldots$ (see Fig. 1). According to our general procedure, we shall make use of four points, P, B, C, D to attain a precision of order h^2, and we shall exploit the remaining freedom to reach our other objectives.

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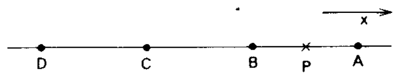

FIG. 1. Moving point on a fixed uniform grid.

According to the method of undetermined coefficients [1] we set

$$\frac{1}{h}(\alpha F_P + \beta F_B + \gamma F_C + \delta F_D) = F'(x_P) + O(h^2), \tag{2}$$

where $F_P = F(x_P)$, etc. Expanding in Taylor series about the point x_P we have from this equation

$$\alpha + \beta + \gamma + \delta = 0, \tag{3a}$$

$$\theta\beta + (1+\theta)\gamma + (2+\theta)\delta = -1, \tag{3b}$$

$$\theta^2\beta + (1+\theta)^2\gamma + (2+\theta)^2\delta = 0, \tag{3c}$$

where

$$\theta = \frac{x_P - x_B}{h},$$

is the quantity which can become undesirably small. Clearly, $0 \leqslant \theta \leqslant 1$. The system (3) has infinitely many solutions. We are interested in that family of solutions which remain bounded as $\theta \to 0$. An immediate consequence of (3b) and (3c) is

$$\beta = -\frac{2 + \theta + (1+\theta)\gamma}{2\theta}.$$

A sufficient condition for β to be bounded is that

$$\gamma = 2[\theta f(\theta) - 1], \tag{4a}$$

where the function $f(\theta)$ is arbitrary but such that $f(0)$ is bounded. In terms of f the solution of (3) is then

$$\alpha = 2\frac{1+f}{2+\theta}, \qquad \beta = \frac{1}{2} - (1+\theta)f, \tag{4b,c}$$

$$\delta = \frac{2 + 3\theta - 2\theta(1+\theta)f}{2(2+\theta)}. \tag{4d}$$

The class of solutions (4) is clearly of the desired form. The residual arbitrariness in the choice of f can be used to confer additional useful properties to the differentiation formula. For instance, one may require the formula to reduce to the standard three-point formula for a uniform grid when $x_P = x_B$ (i.e., $\theta = 0$) or $x_P = x_A$ (i.e., $\theta = 1$). This can be obtained if $\alpha(0) = \frac{3}{2}$, $\beta(0) = 0$, $\gamma(0) = -2$, $\delta(0) = \frac{1}{2}$ and $\alpha(1) = \frac{3}{2}$, $\beta(1) = -2$, $\gamma(1) = \frac{1}{2}$; $\delta(1) = 0$, respectively. All these requirements are satisfied by

$$f(0) = \tfrac{1}{2}, \qquad f(1) = \tfrac{5}{4}. \tag{5}$$

If f is continuous, this choice has the desirable feature that, as P moves from B to A, the influence of point B slowly increases, and correspondingly the influence of D decreases. This avoids the adverse effect of switching abruptly from one triple of points to a different one when θ or $(1-\theta)$ becomes too small. A simple form of f satisfying (5) is a linear function,

$$f(\theta) = \tfrac{1}{2} + \tfrac{3}{4}\theta. \tag{6}$$

With this choice Eqs. (4) become

$$\begin{aligned} \alpha &= \tfrac{3}{2}, & \beta &= -\tfrac{1}{4}\theta(5 + 3\theta), \\ \gamma &= -2 + \theta + \tfrac{3}{2}\theta^2, & \delta &= \tfrac{1}{4}(1-\theta)(2 + 3\theta). \end{aligned} \tag{7}$$

It is obvious that many other useful forms for $f(\theta)$ can be investigated. One possibility would be, for example, to render small the contribution of the terms of order h^3 in some sense suitable for a particular problem. However it appears that the two conditions (5) should always be satisfied to avoid the second difficulty mentioned at the beginning.

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References

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